Kapitza Resistance in Nanocrystalline Yttria-Stabilized Zirconia

SCIENTIFIC ACHIEVEMENT

The grain-size dependence of the thermal conductivity and the magnitude of the interfacial resistance to thermal transport of yttria-stabilized zirconia (YSZ) have been determined for the first time (*Acta Mater.*, **50**, 2309, 2002). Using metal-organic chemical vapor deposition, YSZ coatings were produced with controlled average grain sizes of 10-100 nm. Thermal conductivity measurements were made from 6-480 K using the 3ω technique. Reducing the grain size of YSZ below 40 nm caused a rapid reduction in thermal conductivity, with the thermal conductivity of a 10 nm grain-sized sample only approximately one-third that of a bulk single crystal. The behavior is caused by interfacial resistance to thermal transport (*i.e.*, Kapitza resistance), which, in the presence of an applied heat flux, results in a temperature discontinuity at grain- or phase-boundaries. We derived an analysis technique for determining the magnitude of the Kapitza resistance from the measured grain-size dependence of thermal conductivity. As expected, the temperature dependence of the Kapitza resistance is inversely proportional to that of the specific heat. Orders-of-magnitude differences in the values that we determined for the Kapitza resistance of YSZ compared to the few known values determined in previous studies other materials suggest that our understanding of the factors that determine the magnitude of the interfacial resistance to thermal transport in different materials is at a very early stage. Future systematic studies of Kapitza resistance in materials having different defect concentrations and bulk thermal conductivities are required to obtain a full understanding of thermal transport in nanostructures.

SIGNIFICANCE

Due to the growing interest in the synthesis and properties of nanostructures, as well as the continual trend towards size reduction to the nanometer regime in many industries, obtaining a fundamental understanding of nanoscale heat transfer processes is of critical importance. While previous theoretical work had predicted that interactions between phonons and grain boundaries would significantly decrease thermal transport rates, this study was the first to experimentally verify that the thermal conductivity of a material can have a strong grain-size dependence when the material is synthesized in nanocrystalline form. The recognition that the effects of Kapitza resistance become significant when grain size is reduced to the nanoscale could lead to a new strategy for the development of future-generation thermal barriers based on the use of grain-size-stabilized nanocrystalline microstructures. Future efforts will be devoted to identifying materials that not only have low bulk thermal conductivity, but also large Kapitza resistance; this combination would lead to significantly reduced effective thermal conductivity compared to current-generation thermal barriers.

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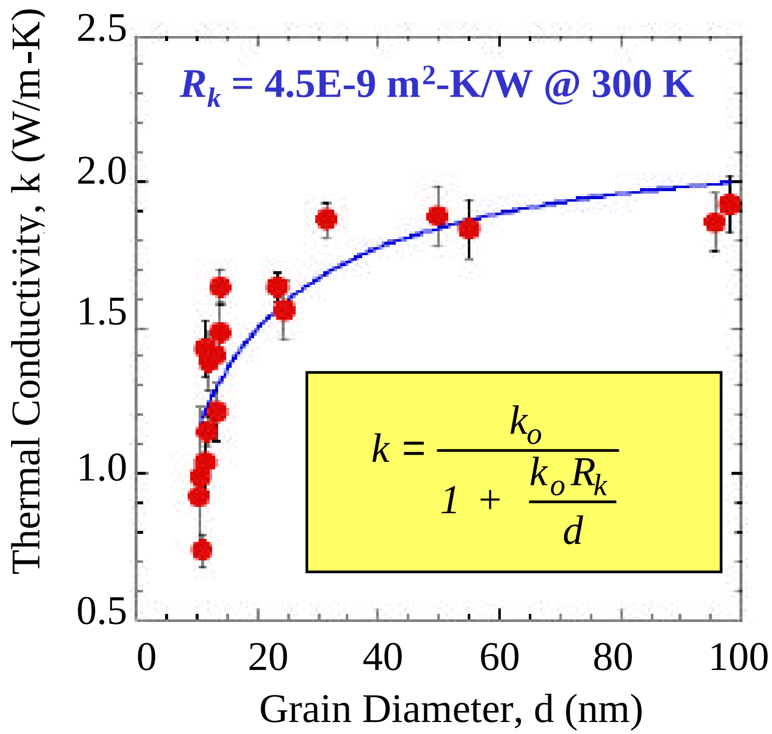

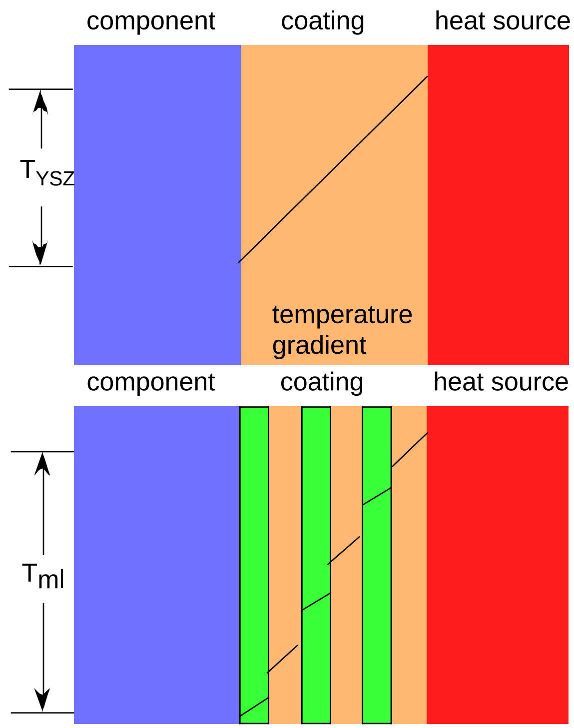

- Reduction of the grain size of yttria-stabilized zirconia (YSZ) below ~ 40 nm results in a strong decrease in thermal conductivity. The Kapitza resistance, $\boldsymbol{R_k}$, is determined from a simple 2-parameter fit to the data.

- Kapitza resistance results in a larger temperature gradient across a material; the use of nanocrystalline materials with large $\boldsymbol{R_k}$ could lead to improved thermal barriers.

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